

1-Nitropropane
108-03-2 | DTXSID1020980

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 9.14e-01

Global applicability domain: Inside

Local applicability domain index: 6.52e-01

Confidence level: 8.38e-01

Nearest Neighbors from the Training Set

Image not found

1-Nitropropane

Measured: 0.87

Predicted: 9.14e-01

Image not found

2-Nitropropane

Measured: 0.93

Predicted: 1.03

Image not found

1-Nitrobutane

Measured: 1.47

Predicted: 1.35

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Propane, 2-methyl-1-nitro-

Measured: 1.40

Predicted: 1.42

Image not found

Allylamine

Measured: 0.03

Predicted: 1.78e-01